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DOCUMENTATION FOR PCDIST, A FORTRAN SUBROUTINE
TO CALCULATE POLLACK-CUZZI SCATTERING

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RESEARCH AND TECHNOLOGY DIRECTORATE

September 1993

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93-28781



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REPORT DOCUMENTATION PAGE			Form Approved OMB No 0704-0188	
<small>Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503.</small>				
1. AGENCY USE ONLY (Leave blank)		2. REPORT DATE 1993 September		3. REPORT TYPE AND DATES COVERED Final, 92 Nov - 93 Mar
4. TITLE AND SUBTITLE Documentation for PCDIST, A Fortran Subroutine to Calculate Pollack-Cuzzi Scattering			5. FUNDING NUMBERS PR-10162622A552	
6. AUTHOR(S) Bottiger, Jerold R.				
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) DIR, ERDEC, ATTN: SCBRD-RTB, APG, MD 21010-5423			8. PERFORMING ORGANIZATION REPORT NUMBER ERDEC-TR-085	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)			10. SPONSORING/MONITORING AGENCY REPORT NUMBER	
11. SUPPLEMENTARY NOTES				
12a. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release; distribution is unlimited.			12b. DISTRIBUTION CODE	
13. ABSTRACT (Maximum 200 words) This report documents a Fortran computer program (PCDIST), which may be used to calculate the light scattering phase function for a distribution of irregularly shaped particles. The subroutine also returns the average particle scattering and absorption cross-sections. PCDIST, which implements the semi-empirical theory of Pollack and Cuzzi, is called from a main program in which the user specifies particle characteristics via a construction called the parameter array. Examples demonstrating the use of the parameter array are given.				
14. SUBJECT TERMS Pollack-Cuzzi Light scattering Irregular particles Aerosol characterization			15. NUMBER OF PAGES 25	
			16. PRICE CODE	
17. SECURITY CLASSIFICATION OF REPORT UNCLASSIFIED	18. SECURITY CLASSIFICATION OF THIS PAGE UNCLASSIFIED	19. SECURITY CLASSIFICATION OF ABSTRACT UNCLASSIFIED	20. LIMITATION OF ABSTRACT UL	

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PREFACE

The work described in this report was authorized under Project No. 10162622A552, Smoke and Obscurants. This work was started in November 1992 and completed in March 1993.

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DOCUMENTATION FOR PCDIST, A FORTRAN SUBROUTINE
TO CALCULATE POLLACK-CUZZI SCATTERING

1. INTRODUCTION

Hodkinson and Greenleaves¹ describe a method, based on classical diffraction and geometric optics, for calculating light scattering from a polydispersion of transparent spheres. The scattered field is treated as arising from three independent processes: diffraction of light rays passing near the spheres; reflection of rays incident on the spheres; and refraction of rays passing through the spheres. The three components are summed without regard to phase relations on the assumption that the size-range of spheres is sufficiently wide to smear out the far field interference effects created within any particular sphere. An exact calculation of the scattering by a polydispersion of spheres can be carried out using Mie theory (in comparisons, the approximation of Hodkinson and Greenleaves holds up well), but the computation, while commonplace today, was challenging for computers of the time, and few tables of Mie results were available then. The purpose of Hodkinson and Greenleaves' work was to provide a method for solving many practical scattering problems while avoiding the use of Mie theory.

Contemporary efforts to calculate light scattering from irregular particles has much in common with the earlier sphere scattering problem. The detailed structure of the scattering pattern produced by any given arbitrary particle in a particular orientation is very difficult today --- usually impossible --- to calculate; in the ordinary circumstance of scattering by a cloud of many rough particles in random orientations, the fine details of the picture should all be averaged out. So rather than attempting a (probably hopeless) detailed calculation for every irregular particle in an ensemble and then averaging the results, one would like to develop and apply a relatively simple procedure that can give the average scattering pattern directly.

Pollack and Cuzzi² suggest using the same three-component approach to nonsphere scattering as had been successfully employed by Hodkinson and Greenleaves to simplify scattering from spheres. They parameterized particle shape in terms of sphericity and surface roughness, and wrote down rules for calculating and combining the diffraction, reflection, and refraction components of scattering. This is an empirical approach, and it succeeds according to whether calculated results and light scattering measurements agree with each other. Pollack and Cuzzi examined experimental light scattering measurements, previously published by a number of authors, and found that their formulae, with appropriately chosen parameter values, could fit

the experimentally determined phase functions of irregular particle systems very well.

To make the Pollack and Cuzzi (P-C) approximation readily available, I have written a Fortran subroutine that can be called by a main program to which the subroutine returns the P-C phase function and average cross-sections for a distribution of irregular particles specified by a "parameter array" in the main program. This report is the documentation for that subroutine, PCDIST. I shall review the P-C approximation more fully, describe how it is implemented in PCDIST, and give a few examples of its use.

2. POLLACK AND CUZZI'S SEMI-EMPIRICAL THEORY

Pollack and Cuzzi's theory treats the scalar (unpolarized) scattering properties of groups of randomly oriented nonspherical particles. They begin with a size parameter distribution $n(X)$ of particles, where the size parameter of a nonspherical particle is equal to the size parameter (circumference to wavelength ratio) of a sphere with equal volume. That part of the distribution with size parameters less than or equal to some breakpoint X_0 is treated as if it consisted of perfect spheres, and Mie theory is applied to determine the phase function and the efficiencies for absorption, scattering, and extinction. Larger particles are handled using the three-component approximation.

The diffraction component of the scattered light produced by an irregular particle of size parameter $X > X_0$ is taken to be the same as that produced by a sphere of size parameter $\sqrt{R}X$, where the factor \sqrt{R} (R is the ratio of the particle's surface area to the equi-volume sphere's surface area) accounts for the irregular particle's greater (on average) projected area. In general, the diffracted intensity distribution about a sphere of size parameter \bar{x} is given by equation 1.³

$$I_D(\theta, \bar{x}) = C_D \frac{\bar{x}^2}{4\pi} \left[\frac{2J_1(\bar{x} \sin \theta)}{\bar{x} \sin \theta} \right]^2 k \quad (1)$$

where

$$k = \frac{1}{2}(1 + \cos^2 \theta). \quad (2)$$

C_D is a normalization constant, chosen so that

$$\int_{4\pi} I_D d\Omega = 2\pi \int_0^\pi I_D \sin\theta d\theta = 4\pi. \quad (3)$$

Pollack and Cuzzi assume that the geometrical optics expression for external reflection from large spheres applies also to all irregular particles with $X > X_0$. That expression is

$$I_R = \frac{1}{2} C_R \left\{ \frac{\sin(\frac{\theta}{2}) - [|\tilde{m}|^2 - 1 + \sin^2(\frac{\theta}{2})]^{\frac{1}{2}}}{\sin(\frac{\theta}{2}) + [|\tilde{m}|^2 - 1 + \sin^2(\frac{\theta}{2})]^{\frac{1}{2}}} \right\}^2 + \frac{1}{2} C_R \left\{ \frac{|\tilde{m}|^2 \sin(\frac{\theta}{2}) - [|\tilde{m}|^2 - 1 + \sin^2(\frac{\theta}{2})]^{\frac{1}{2}}}{|\tilde{m}|^2 \sin(\frac{\theta}{2}) + [|\tilde{m}|^2 - 1 + \sin^2(\frac{\theta}{2})]^{\frac{1}{2}}} \right\}^2 \quad (4)$$

where \tilde{m} is the complex refractive index, and C_R is a normalization constant so that I_R also satisfies equation 3. The two terms represent reflection of parallel and perpendicular polarizations, respectively.

These first two components are the same as those Hodgkinson and Greenleaves used in their approximation for scattering from dielectric spheres. Irregular particle scattering is distinguished from sphere scattering in Pollack and Cuzzi's treatment of the transmitted (i.e., refracted) component of the scattered light. In their scheme, the angular redistribution of light having entered the particle is governed by an empirical law,

$$I_T = C_T \exp(1 + b\theta) \quad (5)$$

where, again, C_T is a normalization constant. The empirical parameter b can be related to another constant, G , by

$$G \equiv \frac{\int_0^{\frac{\pi}{2}} I_T d\theta}{\int_{\frac{\pi}{2}}^\pi I_T d\theta}, \quad (6)$$

which relates the energy reradiated into the forward hemisphere to that reradiated into the back hemisphere. For smooth particles that do not deviate the incident light very much, G is

large, ~ 10 ; whereas, for very rough particles that redistribute the light more uniformly, G is small, ~ 1 . Pollack and Cuzzi do not suggest any quantitative means for assigning a value to G from an examination of the irregular particles; in fact, G is principally used as a fudge-factor to bring about agreement between measured and calculated phase functions.

The scattering efficiency associated with each of the three components must be specified so they may be properly weighted when summed. Consider a single irregular particle (or infinitesimally narrow range) of size parameter X ($> X_0$). The diffraction efficiency is taken to be exactly unity ($Q_D = 1$). That is, it is assumed that any large irregular particle diffracts an amount of energy equal to that falling on its (average) physical cross-section. The efficiency factor for external reflection is $Q_R = \{1/C_R\}$ where C_R is the normalization factor in equation 4. Finally, the scattering efficiency for the transmitted component is given by

$$Q_T = Q_S - Q_D - Q_R \quad (7)$$

where Q_S is the Mie scattering efficiency for the equivalent volume sphere. The total scattering efficiency for the large particle is taken to be RQ_S (because the total scattering cross-section should be proportional to the irregular particle's projected surface area). The absorption efficiency for a large particle is just Q_A , the Mie absorption efficiency for an equivalent volume sphere, unless the particle is highly absorbing ($2mX > 1$), in which case, an extra factor R is also included.

The composite normalized phase function for a large irregular particle is given by

$$PF = I_D \frac{Q_D}{Q_S} + I_R \frac{Q_R}{Q_S} + I_T \frac{Q_T}{Q_S} \quad (8)$$

3. SUBROUTINE PCSING AND ITS DAUGHTERS

The Fortran program PCDIST that implements the P-C approximation is diagramed in Figure 1. The name PCDIST is used to refer both to the entire collection of subroutines shown in the figure and to the uppermost level subroutine that interacts directly with the user's main program. The program structure is best explained by starting in the middle, with PCSING.

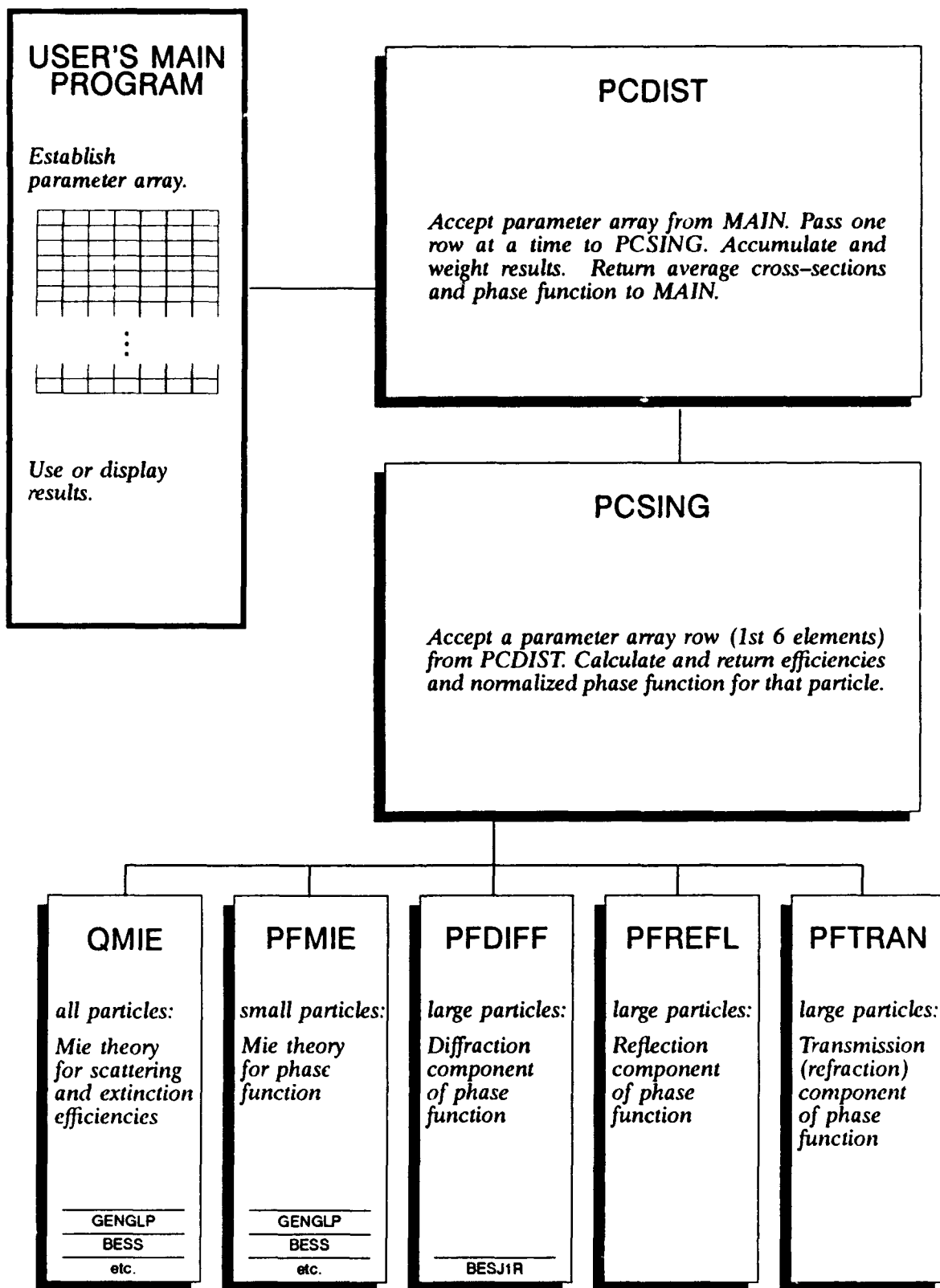


Figure 1. Relationships Among Subroutines Comprising PCDIST

PCSING controls the calculation of the normalized phase function and scattering and absorption efficiencies for a single particle. The required parameters (X , CMR , CMI , R , $X0$, and G) are passed in the argument list of the calling statement within PCDIST. The values CMR and CMI are the real and imaginary parts of the particle refractive index; the other parameters were defined in the previous section. Also passed are $DELTHA$, the increment between scattering angles at which the phase function is to be evaluated, and the closely related $NANG$, the number of angles between 0 and 180°, inclusive, at which the phase function is to be evaluated.

The particle size parameter X is compared to the critical size $X0$; if X is smaller then the subroutines, $QMIE$ and $PFMIE$ are called, in turn, to calculate the particle's efficiencies and phase function as if it were a perfect sphere. Both subroutines are adapted from the excellent programs published by Barber and Hill.⁴ $QMIE$ comes from their program S1, and $PFMIE$ is adapted from their program S3. Both of these Mie subroutines call a number of other subroutines as they proceed; all are included in the PCDIST package.

If X is greater than $X0$, $QMIE$ is still called to obtain the Mie efficiencies; but, the phase function is calculated with the help of three new subroutines. $PFDIFF$ is called for the diffraction part of the phase function, as in equation 1. The quantity $[J_1(z)/z]$ is approximated, very accurately for all z , using the algorithm by Press⁵ for $J_1(z)$. Actually, the diffracted light expressed in equation 1 is symmetric around 90° and peaks equally strongly in the backward and forward directions, which is nonsense. Therefore, I cut the diffracted component off after 90°. That cutoff may put a small nonphysical kink in the phase function curve at 90°, depending on the intensity of the diffraction component at cutoff. To avoid that, I have added an extra $\cos(\theta)$ factor to the expression for I_D . It has no significant effect at small scattering angles but insures that the diffracted component goes smoothly to 0 at 90°. $PFDIFF$ returns to PCSING a 1-d array of numbers (PFD), which are the diffraction phase function values (except for the normalization constant) at all desired angles from 0 to 90°, and it returns the normalization constant, called CDD here. The CDD constant could be multiplied against each number in PFD to return the normalized phase function; but, to save some time, that multiplication is performed later in PCSING in conjunction with Q-weighting and summing the three components.

The reflection component is calculated with $PFREFL$, which proceeds exactly as specified by equation 4. It returns the array PFR , with unnormalized reflection phase function components from 0 to 180° in steps of $DELTHA$, and the normalization constant CDR . Notice that the returned values depend only on the particle refractive index and no other parameters.

Frequently, it should be the case that all of the particles in a distribution of interest have the same refractive index, and a lot of computer time could be wasted recalculating exactly the same reflection result each time a new particle from the distribution is handed to PCSING. Therefore, we use the Fortran SAVE statement to cause PCSING to keep copies of PFR and CDR in static storage, along with the refractive index values, renamed CMROLD and CMIOLD. Each time PCSING is called, the new values CMR and CMI are checked against the old saved ones; if there is no difference, PFREFL is not called. Instead, the previously calculated PFR and CDR are simply reused.

The transmitted component is evaluated in the subroutine PFTRAN. Because of the simple form assumed for I_T , the normalization factor in this case can be written analytically. The condition

$$\int_{4\pi} I_T d\Omega = 2\pi \int_0^\pi C_T \exp(1 + b\theta) \sin \theta d\theta = 4\pi \quad (9)$$

yields

$$C_T = \frac{2}{e \int_0^\pi e^{b\theta} \sin \theta d\theta}. \quad (10)$$

The integral in the denominator can be looked up.⁶ After some algebra, we may write for the normalized transmitted component

$$I_T = \frac{2(b^2 + 1)}{e^{b\pi} + 1} e^{b\theta} \quad (11)$$

However, it is G , not b , which is the user-specified parameter. The relationship between them is discovered by substituting equation 5 into equation 6. One finds then that

$$b = \frac{-2 \ln G}{\pi} \quad (12)$$

Subroutine PFTRAN uses equations 12 and 11 to return a 1-d array, PFT, containing the normalized phase function at angles between 0 and 180° in steps of DELTHA.

Like PFREFL, PFTRAN depends only on a parameter (G), which may be constant for the entire distribution of particles. So again, to avoid unnecessary calculations, a copy of PFT and the old value of G is saved in PCSING, and PFT is recalculated for new particles only if the value of G is changed.

PCSING assembles the final normalized phase function (PFS) array by calculating for each angle, indexed by I,

$$PFS(I) = \frac{CDD}{QSCA} PFD(I) + QR \frac{CDR}{QSCA} PFR(I) + \frac{QT}{QSCA} PFT(I) \quad (13)$$

where QSCA is the Mie scattering efficiency returned by QMIE. Finally, the particle's total scattering efficiency is given as $\sqrt{R} \times QSCA$, and its absorption efficiency is either QABS (returned by QMIE) or $\sqrt{R} \times QABS$, depending on 2X CMI.

It is easy to temporarily modify PCDIST so that it writes a file to disk containing the normalized total phase function and the three (normalized) partial phase functions that went into it --- as functions of scattering angle. A plot of those data helps one to visualize the P-C approximation. For example, Figure 2 shows such a plot for a relatively small rough particle. Its P-C parameters were: $X = 8$, $CMR = 1.5$, $CMI = 0.05$, $X0 = 3$, $R = 1.4$, and $G = 2$. Figure 3 shows a particle of the same shape and material but larger with a smoother surface: $X = 30$ and $G = 8$, with the other parameters as shown in Figure 2. Notice the higher frequency oscillations and the steeper transmission slope in Figure 3 compared to Figure 2.

4. SUBROUTINE PCDIST AND THE PARAMETER ARRAY

PCDIST is the top level of the subroutine; it gets information about the distribution of irregular particles from the user's main program, calls PCSING repeatedly to get the scattering properties of each representative particle of the distribution, and combines the accumulated results to construct the scattering properties (phase function and cross-sections) of the distribution.

Data describing the cloud of irregular particles is transferred by way of a parameter array, which the user must construct in his main program; the parameter array name is passed

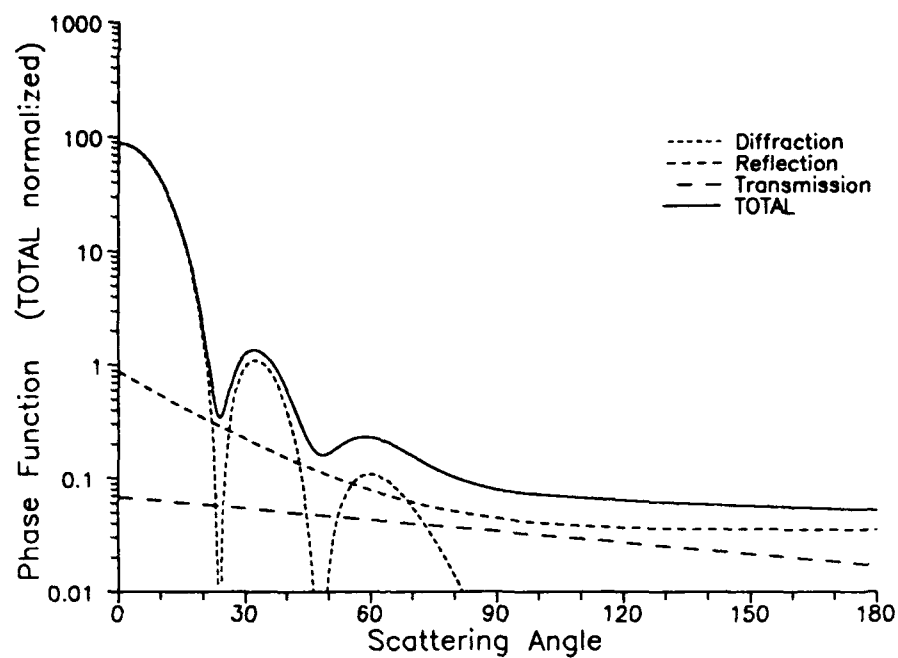


Figure 2. P-C Phase Function when $X = 8$ and $G = 2$

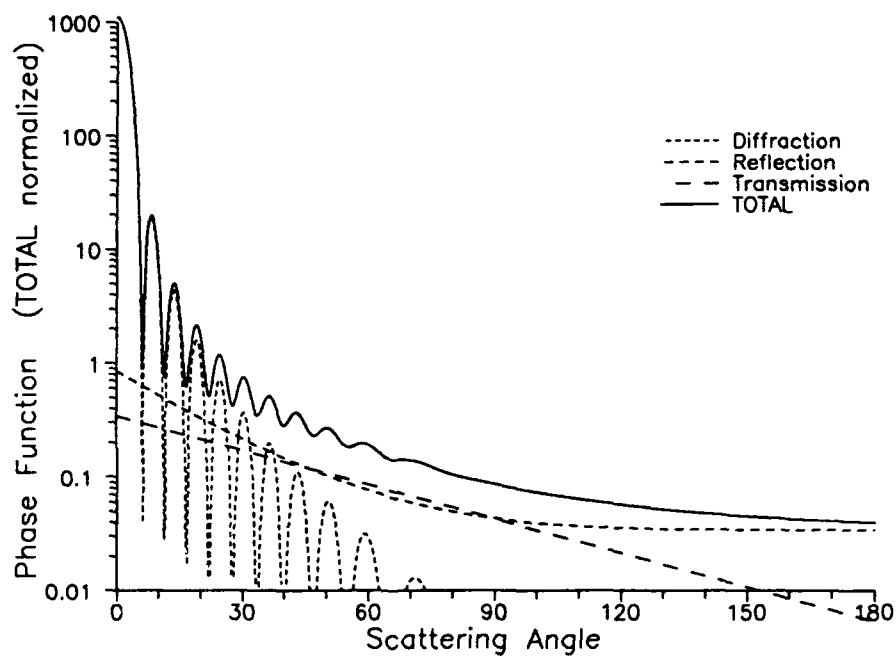


Figure 3. P-C Phase Function when $X = 30$ and $G = 8$

to PCDIST in the calling statement argument list. The array must have seven columns and one or more rows. Each row either represents one particle or one type of particle in the distribution. The first six columns contain the Pollack-Cuzzi parameters already discussed --- in order: X , CMR , CMI , X_0 , R , and G . The seventh column value tells what fraction of the cloud's particles are represented by the particle described in that row. Usually, the seventh column is just the particle size distribution function evaluated at the row's X value; however, sometimes more complicated expressions will be appropriate. The parameter array is a powerful and flexible structure that allows one to solve almost any scattering problem of this type with a few simple lines of code.

When PCDIST is called, the argument list must also contain $NROWS$, the number of rows in the parameter array, and $DELTHA$, the step size in degrees at which the phase function is desired. Typically, about 100 rows should suffice for specifying a particle distribution, in the sense that a higher resolution specification using more rows will not yield a significantly different result. The current version of PCDIST is dimensioned for a maximum of 5000 rows, which should cover any situation. That dimension can be easily changed; if it is made too much larger, a user's program linked with PCDIST will not fit on a DOS machine. The smallest value for $DELTHA$ allowed in the current version is 0.05° , but it is difficult to imagine the need for such a fine scale. To shorten execution time, one should set $DELTHA$ no smaller than is needed to get phase function values at whatever particular angles are desired. However, $DELTHA$ should not be too large either ($> 10^\circ$) because $DELTHA$ sets the quadrature size in evaluating the phase function normalizations, and errors can creep in if the scale becomes too coarse. $DELTHA = 1^\circ$ will work well in most circumstances; in any event, $DELTHA$ must always be chosen such that $180/DELTHA$ is an integer.

PCDIST calls PCSING $NROWS$ times, getting back $NROWS$ individual phase functions and absorption and scattering efficiencies. Each phase function is weighted according to its contribution to the total scattering; then, the functions are all added together. Finally, the sum of the weighted phase functions is normalized. The weighting factor for each contribution is the product of the scattering cross-section (which is proportional to X^2 times the scattering efficiency) times the column seven factor (the relative number of particles of that type). The weighted average scattering and absorption cross-sections are similarly calculated.

5. EXAMPLES

A few examples of main programs that call PCDIST should clarify how the parameter array is to be used. The first is quite simple.

5.1 Example 1.

Calculate the phase function for a cloud of irregular particles with a log-normal size distribution. The material of which the particles are made has a refractive index of $1.45 + 0.05i$, and the other Pollack-Cuzzi parameters (valid for all the particles) are $X_0 = 3$, $R = 1.3$, and $G = 5$. The size distribution peaks at $X = 5$, and the sigma is 0.2.

Figure 4 displays a code to accomplish example 1. The parameter array (called PAR here) and phase function array (PF) must always be dimensioned exactly as shown in line six to agree with their dimensions in PCDIST.

A log-normal distribution $n(X)$ is given by

$$n(X) \propto \frac{1}{(SG) X} \exp\left(\frac{-(\ln X - \ln(XM))^2}{2 (SG)^2}\right) \quad (14)$$

where XM is the geometric mean size, and SG is the geometric standard deviation. We consider particles with sizes up to three geometric standard deviations from the mean and divide that range into 200 intervals (lines 19-22).

The parameter array PAR, which in this case will use only 201 of the 5000 rows dimensioned to it, is set up in lines 24-33. The first column of PAR holds the 201 values of X , and the seventh holds the corresponding probabilities, from equation 14. It is not necessary to normalize the probability distribution; numerical normalization of the final phase function will be done by PCDIST and will be unaffected by any constant factors in distributions such as equation 14.

This program writes the scattering and absorption cross-sections to the screen (since particle size parameter was given, a wavelength must yet be specified to convert the cross-sections into actual areas) and writes files listing the calculated phase function and the distribution function used (equation 14). Figure 5 shows plots of the program output files, PHASFUNC.DAT and DISTFUNC.DAT.

PROGRAM		EX1.FOR		
VERSION		Mon Mar 01 08:16:58 1993		
LINE #	SOURCE CODE		PAGE 1	
1	PROGRAM EX1			
2	c	A main program to call pcdist for a log-normal		
3	c	size distribution of particles.		
4				
5	REAL*8 XLOW, XHIGH, DELX, XM, SG, CMR, CMI, XO, R, G			
6	REAL*8 PAR(5000,7), PF(0:3600), CSCA, CABS, DELTHA			
7	INTEGER I, J, NROWS, NANG			
8				
9	CMR = 1.45			
10	CMI = 0.05			
11	XO = 3			
12	R = 1.3			
13	G = 5			
14	DELTHA = 1.0			
15	NANG = 181			
16	XM = 5			
17	SG = .2			
18				
19	XHIGH = EXP(LOG(XM) + 3.0*SG)			
20	XLOW = EXP(LOG(XM) - 3.0*SG)			
21	DELX = (XHIGH-XLOW)/200.			
22	NROWS = 201			
23				
24	DO 30 I=1,NROWS			
25	X=XLOW+DELX*REAL(I-1)			
26	PAR(I,1) = X			
27	PAR(I,2) = CMR			
28	PAR(I,3) = CMI			
29	PAR(I,4) = XO			
30	PAR(I,5) = R			
31	PAR(I,6) = G			
32	PAR(I,7) = (1./(SG*X))*EXP(-(LOG(X)-LOG(XM))**2/(2.*SG**2))			
33	30 CONTINUE			
34				
35	CALL PCDIST(NROWS, PAR, DELTHA, CSCA, CABS, PF)			
36				
37	WRITE(*,3) CSCA			
38	3 FORMAT(' CSCA = ',F8.2,2X,'times lambda squared')			
39	WRITE(*,4) ABS(CABS)			
40	4 FORMAT(' CABS = ',F8.2,2X,'times lambda squared')			
41				
42	OPEN(UNIT=11, FILE='PHASFUNC.DAT')			
43	DO 40 J=0,(NANG-1)			
44	40 WRITE(11,21) DELTHA*REAL(J), PF(J)			
45	21 FORMAT(F8.2, E12.4)			
46	CLOSE(11)			
47				
48	OPEN(UNIT=12, FILE='DISTFUNC.DAT')			
49	DO 50 I=1,NROWS			
50	50 WRITE(12,22) PAR(I,1), PAR(I,7)			
51	22 FORMAT(F8.3, E12.4)			
52	CLOSE(12)			
53	STOP			
54	END			

Figure 4. Fortran Code to Solve Example 1

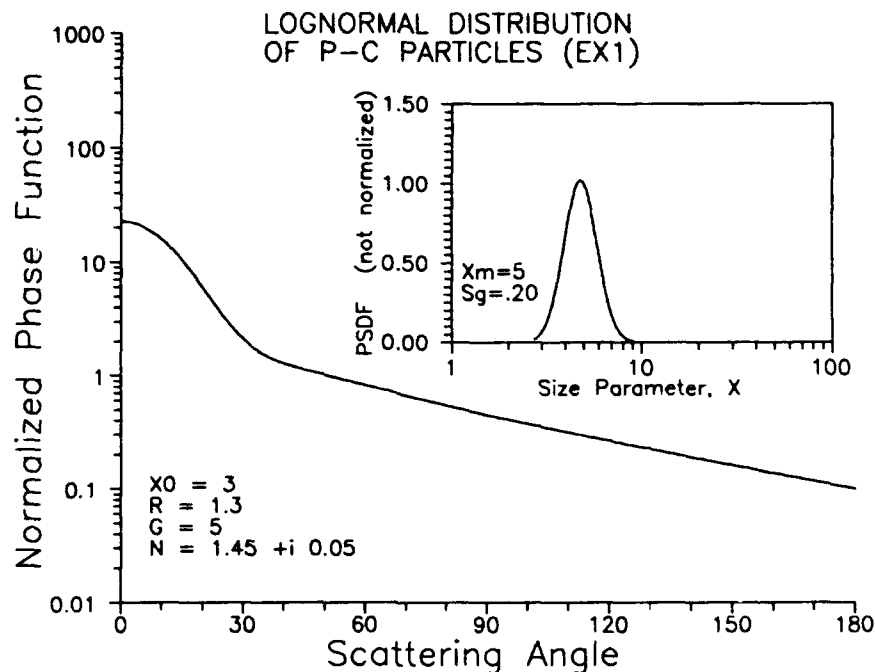


Figure 5. Plot of Data Generated by Running EX1.FOR

5.2 Example 2.

Suppose a cloud consists of uniform NaCl cubic particles, 2.0μ on edge (as might be generated by a vibrating orifice aerosol generator loaded with saltwater). What is the phase function of this aerosol when illuminated by an incandescent lamp with a color temperature of 6000 K?

In this case, the particles all have the same physical size, but a distribution in the size parameter arises from the broad spectrum of the incident wavelengths. Several of the parameters to be loaded into the parameter array are functions of wavelength. A sphere with diameter

$$d = 2\sqrt[3]{\frac{3}{4\pi}} a \quad (15)$$

has the same volume as a cube with side a . The size parameter of the equivalent volume sphere is

$$X = \frac{\sqrt[3]{6\pi^2} a}{\lambda} \quad (16)$$

and the ratio of surface areas is

$$R = \frac{6}{4\pi(\frac{3}{4\pi})^{\frac{2}{3}}} = 1.2407 \quad (17)$$

The lamp spectral distribution may be taken from Planck's Law which, for $T = 6000$ K and λ in microns, has the form

$$I(\lambda) \propto \frac{1}{\lambda^5(e^{\frac{24}{\lambda}} - 1)} \quad (18)$$

The relative number of particles of each size parameter (i.e., column seven in the parameter array) comes from this expression. Almost all of the lamp's energy is radiated at wavelengths between 0.2 and 2μ , which will be taken as the limits of the spectrum. We (rather arbitrarily) divide this range into 60 equal intervals and look at 61 particle types.

Another wrinkle in this example is that the refractive index is different for each particle type; it varies with wavelength. The real refractive index for NaCl over the range of interest may be approximated (with λ in microns) by

$$CMR = 1.52122 + \frac{.01095}{\lambda^2} - \frac{.00000683}{\lambda^4} \quad (19)$$

obtained by fitting the Cauchy dispersion formula with data from the AIP handbook.⁷ The imaginary part is zero.

Figure 6 is a simple program that loads a parameter array in accordance with equations 16-19 and writes a file of the phase function values every 1° . In Figure 7, the phase function is plotted.

5.3 Example 3.

In this last example, the same conditions in example 2 hold, except that now we also include a distribution in the physical sizes of the salt cubes. Suppose the cube lengths are normally distributed, with a mean size of 2.0μ and a standard

PROGRAM		EX2.FOR
VERSION		Fri Feb 26 18:28:26 1993
LINE #	SOURCE CODE	PAGE 1
1	PROGRAM EX2	
2	c Main program example 2.	
3		
4	REAL*8 PAR(5000,7), PF(0:3600), CSCA, CABS, DELTHA, WAV	
5	INTEGER I, J, NROWS, NANG	
6		
7	DELTHA = 1	
8	NANG = 181	
9	NROWS = 61	
10		
11	DO 10 I=1,NROWS	
12	WAV = .20 + REAL(I-1)*.03	
13	PAR(I,1) = 7.794/WAV	
14	PAR(I,2) = 1.52122 + .01095/WAV**2 - .00000683/WAV**4	
15	PAR(I,3) = 0.0	
16	PAR(I,4) = 8	
17	PAR(I,5) = 1.2407	
18	PAR(I,6) = 6	
19	PAR(I,7) = 1/(WAV**5 * (EXP(2.4/WAV) -1))	
20	10 CONTINUE	
21		
22	CALL PCDIST(NROWS, PAR, DELTHA, CSCA, CABS, PF)	
23		
24	OPEN(UNIT=11, FILE='PHASFUNC.DAT')	
25	DO 40 J=0,(NANG-1)	
26	40 WRITE(11,21) DELTHA*REAL(J), PF(J)	
27	21 FORMAT(F8.2, E12.4)	---
28	CLOSE(11)	
29	STOP	
30	END	

Figure 6. Fortran Code to Solve Example 2

deviation of 0.3μ , from 1.0 to 3.0μ . The probability that a random cube has an edge of length a is proportional to

$$P \propto \exp\left(-\frac{1}{2}\left(\frac{a - 2.0}{.3}\right)^2\right) \quad (20)$$

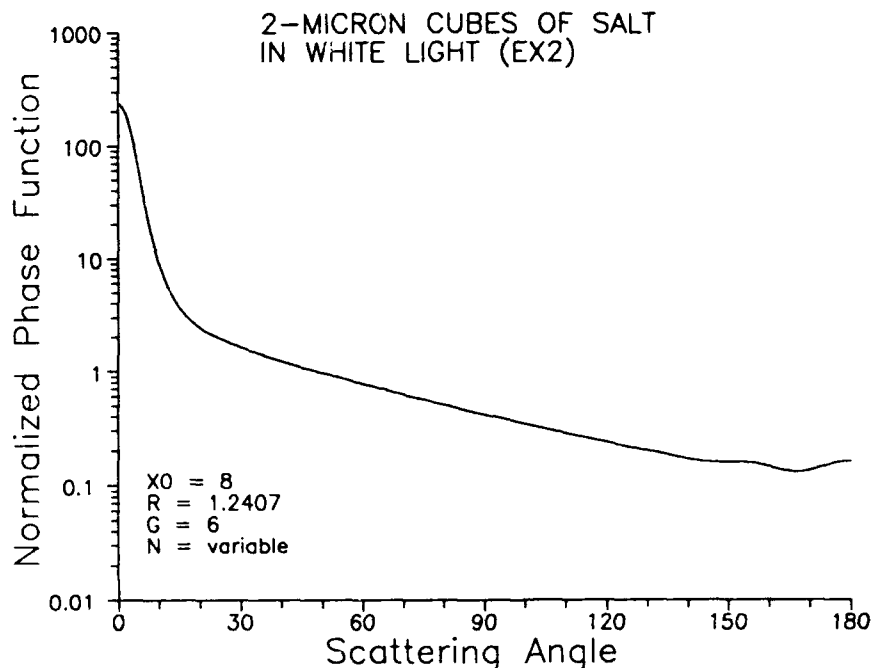


Figure 7. Plot of Data Generated by Running EX2.FOR

We divide the particle size range evenly from 1.0 to 3.0μ in steps of 0.04μ and must now run over all 51 particle sizes at each of the 61 wavelengths. This is done in the code of Figure 8, where $61 \times 51 = 3111$ rows of particle types are defined with a nested do-loop. The weight given to each type (column seven) is just the product of the wavelength distribution and the particle size distribution functions. As it happens, the phase function calculated for example 3 is only very slightly different from that of example 2 because smoothing over size parameters is virtually complete from the broad wavelength distribution alone.

6. CONCLUSION

I have documented the operation of a subroutine, PCDIST, which may be called from a Fortran program to calculate

PROGRAM		EX3.FOR
VERSION		Fri Feb 26 18:28:28 1993
LINE #	SOURCE CODE	PAGE 1
1	PROGRAM EX3	
2	c Main program example 3.	
3		
4	REAL*8 PAR(5000,7), PF(0:3600), CSCA, CABS, DELTHA, WAV, A	
5	INTEGER I, J, K, NROWS, NANG	
6		
7	DELTHA = 1	
8	NANG = 181	
9	NROWS = 3111	
10		
11	DO 10 I=1,61	
12	WAV = .20 + REAL(I-1)*.03	
13	DO 20 K=1,51	
14	A = 1.0 + REAL(K-1)*.04	
15	PAR((I-1)*51+K,1) = 3.897*A/WAV	
16	PAR((I-1)*51+K,2) = 1.52122 + .01095/WAV**2 - .00000683/WAV**4	
17	PAR((I-1)*51+K,3) = 0.0	
18	PAR((I-1)*51+K,4) = 8	
19	PAR((I-1)*51+K,5) = 1.2407	
20	PAR((I-1)*51+K,6) = 6	
21	PAR((I-1)*51+K,7) = (1/(WAV**5*(EXP(2.4/WAV)-1)))	
22	& *EXP(-.5*((A-2.0)/.3)**2)	
23	20 CONTINUE	
24	10 CONTINUE	
25		
26	CALL PCDIST(NROWS, PAR, DELTHA, CSCA, CABS, PF)	
27		
28	OPEN(UNIT=11, FILE='PHASFUNC.DAT')	
29	DO 40 J=0,(NANG-1)	
30	40 WRITE(11,21) DELTHA*REAL(J), PF(J)	
31	21 FORMAT(F8.2, E12.4)	
32	CLOSE(11)	
33	STOP	
34	END	

Figure 8. Fortran Code to Solve Example 3

the cross sections and phase function of a cloud of irregular particles, using the Pollack and Cuzzi approximations. The subroutine interacts with the programmer's main program through a structure called the parameter array, which specifies the particles' properties through rules explained in this report. Finally, to elucidate the use of the parameter array, we have given some bare-bones examples of main programs calling PCDIST.

LITERATURE CITED

1. Hodkinson, J.R., and Greenleaves, I., "Computation of Light Scattering and Extinction by Spheres According to Diffraction and Geometric Optics, and Some Comparisons with the Mie Theory," *J. Op. Soc. Am.* Vol. 53, No. 5, pp 577-588 (1962).
2. Pollack, J.B., and Cuzzi, J.N., "Scattering by Nonspherical Particles of Size Comparable to a Wavelength: A New Semi-Empirical Theory and Its Application to Tropospheric Aerosols," *J. Atmos. Sci.* Vol. 37, pp 868-881 (1980).
3. Born, M., and Wolf, E., *Principles of Optics*, Fifth ed., p 396, Pergamon Press, New York, NY, 1975.
4. Barber, P.W., and Hill, S.C., *Light Scattering by Particles: Computational Methods*, World Scientific Publishing Company, Teaneck, NJ, 1990.
5. Press, W.H., et al., *Numerical Recipes*, Cambridge University Press, Cambridge, MA, 1987.
6. Gradshteyn, I.S., and Ryzhik, I.V., *Tables of Integrals Series and Products*, (Formula 2.662-1), Academic Press, New York, NY, 1965.
7. Gray, D.E., Ed., *American Institute of Physics Handbook*, McGraw-Hill Book Company, New York, NY, 1972.